

AD-A184 282

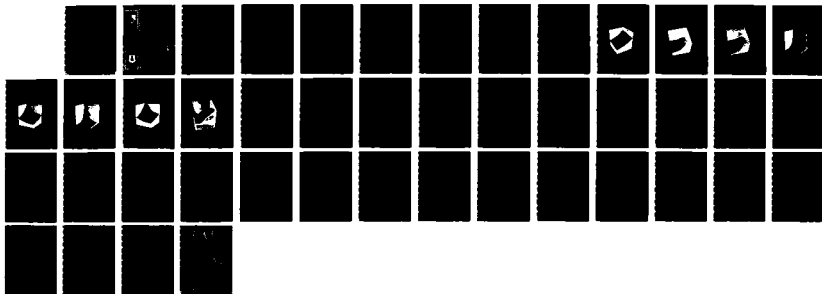
TEMPERATURE-COMPOSITION SURFACES FOR PHYSICAL
PROPERTIES OF ALUMINUM CHLO (U) FRANK J SEILER
RESEARCH LAB UNITED STATES AIR FORCE ACADEMY C

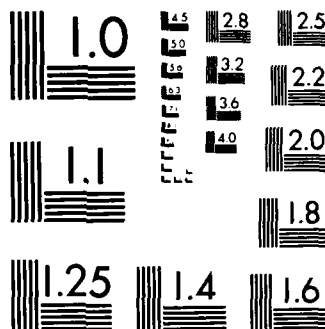
1/1

UNCLASSIFIED

A A FANNIN ET AL JUL 86 FJSRL-TR-86-0004 F/G 7/4

NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

FJSRL-TR-86-0004

RTM: FILE COPY

1

AD-A184 282



FRANK J. SEILER RESEARCH LABORATORY

**TEMPERATURE-COMPOSITION SURFACES FOR
PHYSICAL PROPERTIES OF ALUMINUM CHLORIDE-
1-METHYL-3-ETHYLIMIDAZOLIUM CHLORIDE
ROOM TEMPERATURE MOLTEN SALTS**

LT COL ARMAND A. FANNIN, JR.

DR. JOHN S. WILKES

**DTIC
ELECTE
SEP 03 1987**
S
E

**APPROVED FOR PUBLIC RELEASE;
DISTRIBUTION UNLIMITED.**

July 1986

**AIR FORCE SYSTEMS COMMAND
UNITED STATES AIR FORCE**



87 9 1 333

FJSRL-TR-86-0004

This document was prepared by the Electrochemistry Division, Directorate of Chemical Sciences, Frank J. Seiler Research Laboratory, United States Air Force Academy, CO. The research was conducted under Project Work Unit number 2303-F2-10. Dr. John S. Wilkes was the project scientist.

When U.S. Government drawings, specifications, or other data are used for any purpose other than a definitely related government procurement operation, the government thereby incurs no responsibility nor any obligation whatsoever, and the fact that the government may have formulated, furnished or in any way supplied the said drawings, specifications or other data is not to be regarded by implication or otherwise, as in any manner licensing the holder or any other person or corporation or conveying any rights or permission to manufacture, use or sell any patented invention that may in any way be related thereto.

Inquiries concerning the technical content of this document should be addressed to the Frank J. Seiler Research Laboratory (AFSC), FJSRL/NC, USAF Academy, Colorado Springs, CO 80840. Phone AC 303-472-2655.

This report has been reviewed by the Commander and is releasable to the National Technical Information Service (NTIS). At NTIS it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.



JOHN S. WILKES
Project Scientist



CHESTER J. DYMEK, JR., Lt Col, USAF
Director, Chemical Sciences

KENNETH E. SIEGENTHALER, Lt Col, USAF
Chief Scientist

Copies of this report should not be returned unless return is required by security considerations, contractual obligations, or notice on a specific document.

Printed in the United States of America. Qualified requestors may obtain additional copies from the Defense Documentation Center. All others should apply to:

National Technical Information Service
6285 Port Royal Road
Springfield VA 22161

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified			1b. RESTRICTIVE MARKINGS	
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited.	
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE			5. MONITORING ORGANIZATION REPORT NUMBER(S)	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) FJSRL-TR-86-0004			7a. NAME OF MONITORING ORGANIZATION	
6a. NAME OF PERFORMING ORGANIZATION Frank J. Seiler Research Laboratory		6b. OFFICE SYMBOL (If applicable) FJSRL/NC	7b. ADDRESS (City, State and ZIP Code)	
6c. ADDRESS (City, State and ZIP Code) FJSRL/NC USAF Academy Colorado Springs CO 80840-6528			9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER	
8a. NAME OF FUNDING/SPONSORING ORGANIZATION AF Office of Scientific Rsch		8b. OFFICE SYMBOL (If applicable) AFOSR	10. SOURCE OF FUNDING NOS.	
8c. ADDRESS (City, State and ZIP Code) AFOSR Bldg. 410 Rolling AFB DC 20332		PROGRAM ELEMENT NO. 6,1	PROJECT NO. 2303	TASK NO. F2
11. TITLE (Include Security Classification) Temperature-Composition Surfaces for Phys. Prop. of Alum Chloride - 1-		WORK UNIT NO. 10		
12. PERSONAL AUTHOR(S) Methyl-3-Ethylimid, Chloride Rm, Temp Molten Salts Armand A. Fannin, Jr. and John S. Wilkes				
13a. TYPE OF REPORT Tech Report		13b. TIME COVERED FROM 1 Jun 86 TO 30 Jun 86	14. DATE OF REPORT (Yr., Mo., Day) 86 Jul 02	15. PAGE COUNT 40
16. SUPPLEMENTARY NOTATION				
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
FIELD	GROUP	SUB. GR.	density molten salts	
			viscosity	
			conductivity	
19. ABSTRACT (Continue on reverse if necessary and identify by block number) Density, specific conductivity, equivalent conductivity, absolute viscosity, kinematic viscosity and the Walden product for molten salts composed of aluminum chloride and 1-methyl-3-ethylimidazolium chloride were plotted in three dimensions. The properties were dependent on temperature and composition. ;				
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS <input type="checkbox"/>			21. ABSTRACT SECURITY CLASSIFICATION	
22a. NAME OF RESPONSIBLE INDIVIDUAL JOHN S. WILKES			22b. TELEPHONE NUMBER (Include Area Code) 303-472-2655	22c. OFFICE SYMBOL FJSRL/NC

FJSRL-TR-86-0004

TEMPERATURE - COMPOSITION SURFACES FOR PHYSICAL PROPERTIES
OF ALUMINUM CHLORIDE - 1-METHYL-3-ETHYLIMIDAZOLIUM CHLORIDE
ROOM TEMPERATURE MOLTEN SALTS

Lt Col Armand A. Fannin, Jr.
Dr John S. Wilkes

July 1986

Approved for public release; distribution unlimited

Directorate of Chemical Sciences
The Frank J. Seiler Research Laboratory
Air Force Systems Command
United States Air Force Academy
Colorado Springs, Colorado 80840

LIST OF ILLUSTRATIONS

Figure 1, Density	4
Figure 2, Specific Conductivity	5
Figure 3, Equivalent Conductivity	6
Figure 4, Kinematic Viscosity	7
Figure 5, Log of Kinematic Viscosity.	8
Figure 6, Absolute Viscosity.	9
Figure 7, Log of Absolute Viscosity10
Figure 8, Walden Product.11

INTRODUCTION

Molten salts composed of aluminum chloride and 1-methyl-3-ethylimidazolium chloride are interesting and useful as electrolytes in electrochemical cells and as solvents for a variety of applications. We have reported that the physical properties (density, electric conductivity and viscosity) depend strongly on temperature and melt composition (1). In our original report we plotted the physical properties as conventional two-dimensional graphs, showing the dependence of temperature and compositions separately. In this report we show the properties plotted as three-dimensional surfaces. This treatment of the data make certain trends much easier to visualize. The plots were made possible by the acquisition of the graphics program DISSPLA™.

Accession For	
NTIS GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	

QUALITY
INSPECTED
2

PLOTTING METHOD

DISSPLA™ is a set of FORTRAN calls that provides for the plotting of data or functional surfaces generated in user provided programs. Details about the use and content of DISSPLA™ are contained in the software documentation. The FORTRAN programs written to plot figures 1 - 8 are listed in Appendix A. The essential feature of each is a function that calculates the desired physical property as a function of temperature and composition.

PHYSICAL PROPERTY SURFACES

The functions for the temperature and composition dependencies of the properties used were as reported in reference 1. In summary, the temperature behavior was fitted to a V-T-F model for conductivity and viscosity and to a linear model for density. The composition behavior for all properties was fitted to a complex structural model that is discussed in detail in reference 1. This model allows for the marked change that occurs in some properties at equimolar composition. The equations and fitted parameters are collected in Appendix B. In all plots the temperature is plotted in degrees Celsius and the composition is plotted as mole fraction of aluminum chloride. Superimposed on each surface is a polygon that encloses the area where actual measurements were made.

Density

The density surface is shown in figure 1. The density decreases linearly with temperature at all compositions, however the strength of the dependence varies with composition. The density increases with increasing AlCl_3 mole fraction, as expected.

Electric Conductivity

Both specific and equivalent conductivities were plotted. Specific conductivity is shown in figure 2 and equivalent conductivity is shown in figure 3. The cusp occurring at all temperatures at 0.5 mole fraction is much sharper in specific conductivity as a consequence of the large partial molar volume of AlCl_3 .

Viscosity

Kinematic and absolute viscosity are presented in figures 4-7. For figures 4 and 6 the units are centistokes and centipoise respectively. It may be easily seen that the melt viscosity extends to both higher and lower values than typical values for water. The region of steep increase in viscosity corresponds to the highly structured basic region at low temperatures. To show more detail in the region of lower viscosities, figures 5 and 7 show unitless representations where both viscosities are drawn on a \log_{10} scale.

Walden product

For solutions where the Walden product (equivalent conductivity times the absolute viscosity) is a constant, changes in conductivity may be attributed to only changes in the viscosity. While the theory holds exactly only for infinitely dilute solutions in solvents of differing viscosity, the melts may at least qualitatively be considered a solvent with viscosity a function of the composition. Since concentration of the transporting species changes smoothly and monotonically on each half of the mole fraction diagram, one would expect two monotonically varying Walden product surfaces intersecting at 0.5 mole fraction. The variation from such surfaces drawn in figure 8 gives strong indication of some strong specific interactions or structure in the melts.

REFERENCE

1. Armand A. Fannin, Jr., Danilo A. Floreani, Lowell A. King, John S. Landers, Bernard J. Piersma, Daniel J. Stech, Robert L. Vaughn, John S. Wilkes, and John L. Williams, J. Phys. Chem., **88**, 2614 (1984).

Melt Density

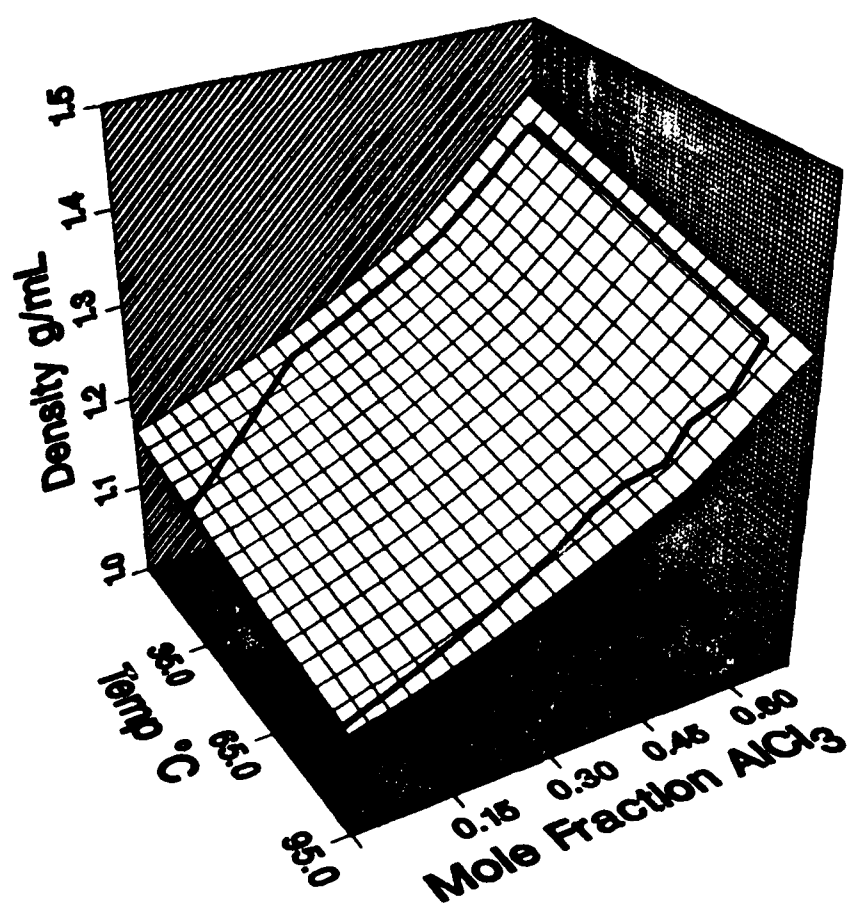


Figure 1

Melt Specific Conductivity

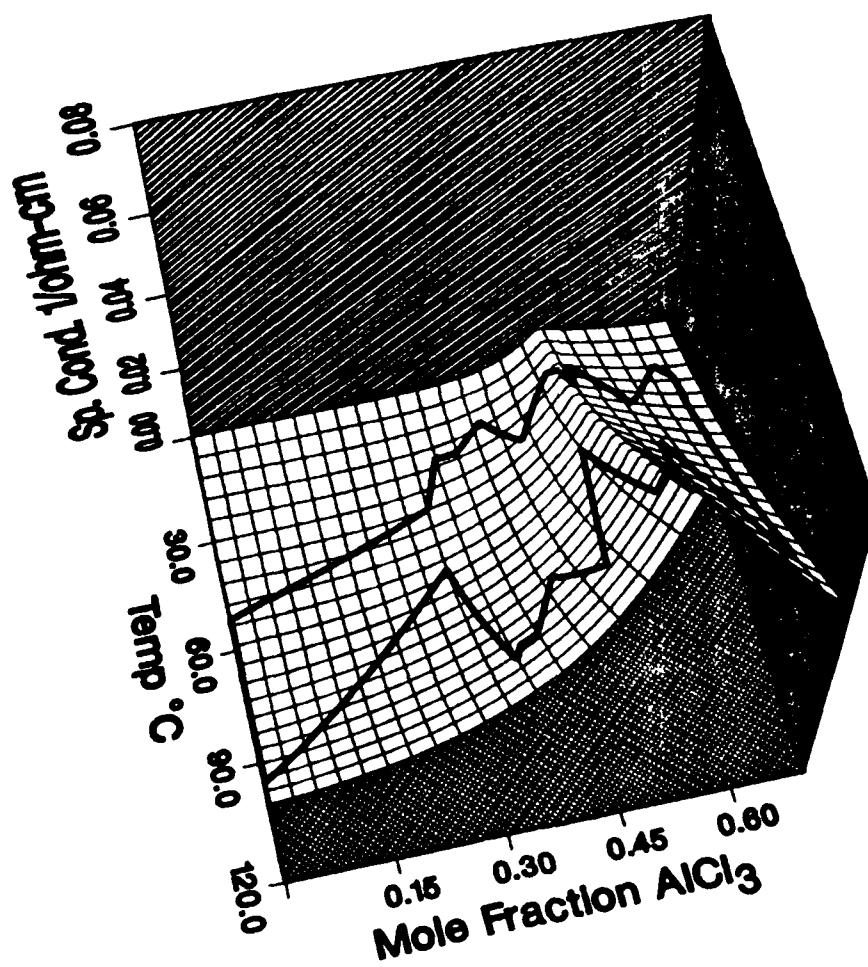


Figure 2

Melt Equiv. Conductivity

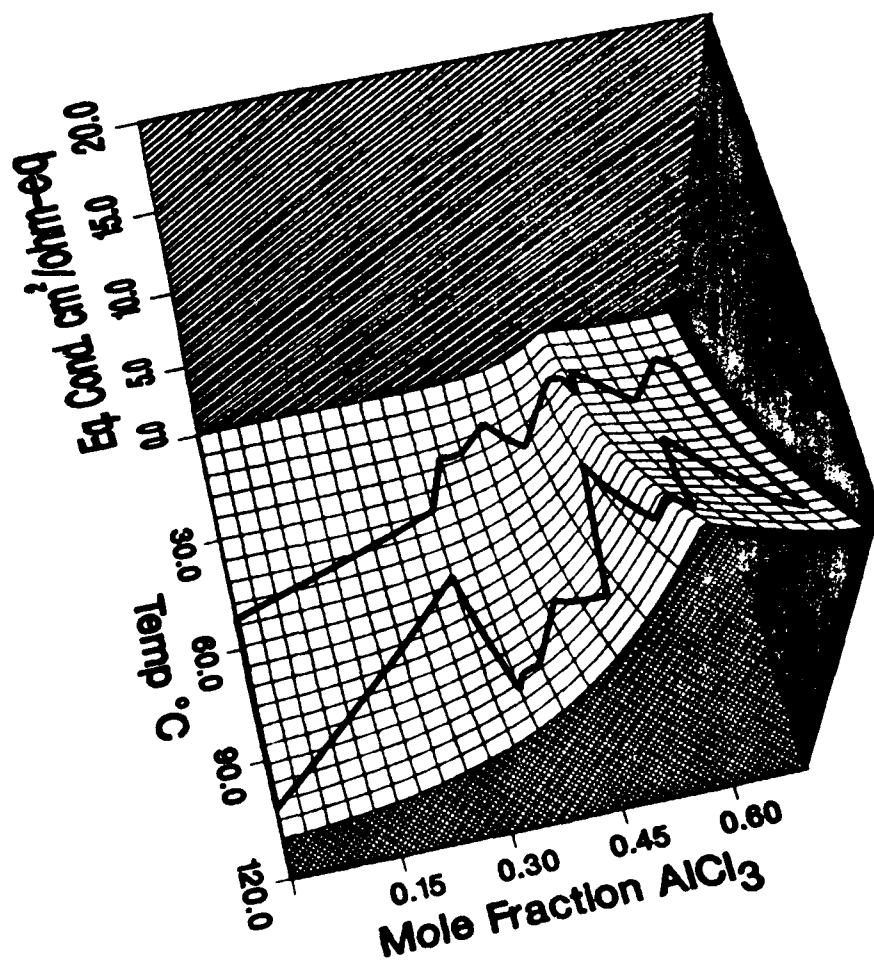


Figure 3

Melt Kinematic Viscosity

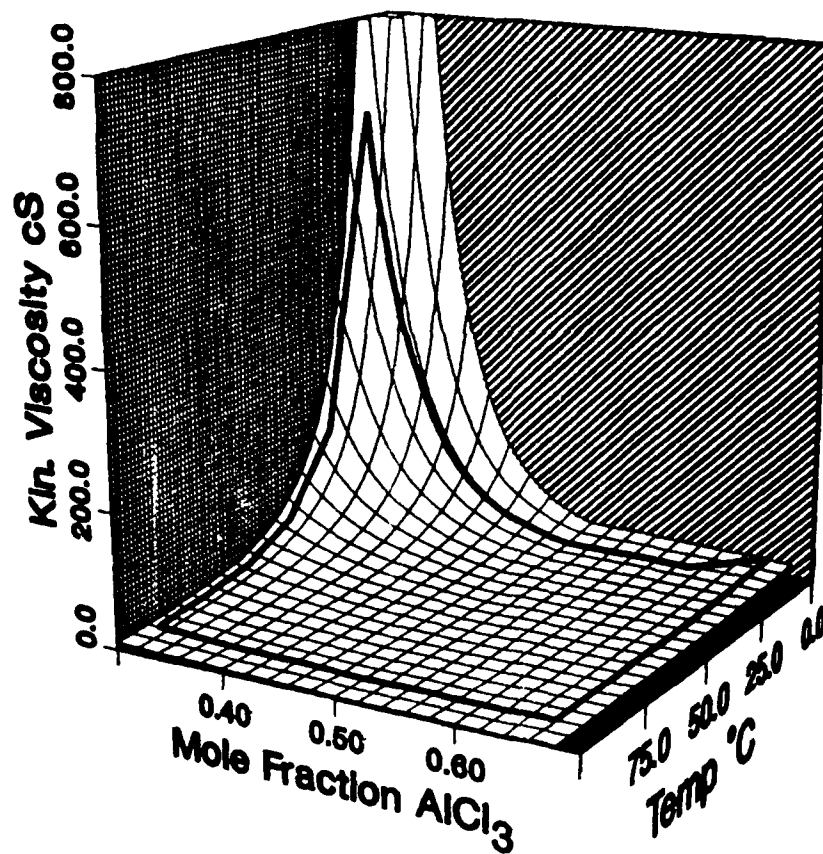


Figure 4

Melt Kinematic Viscosity

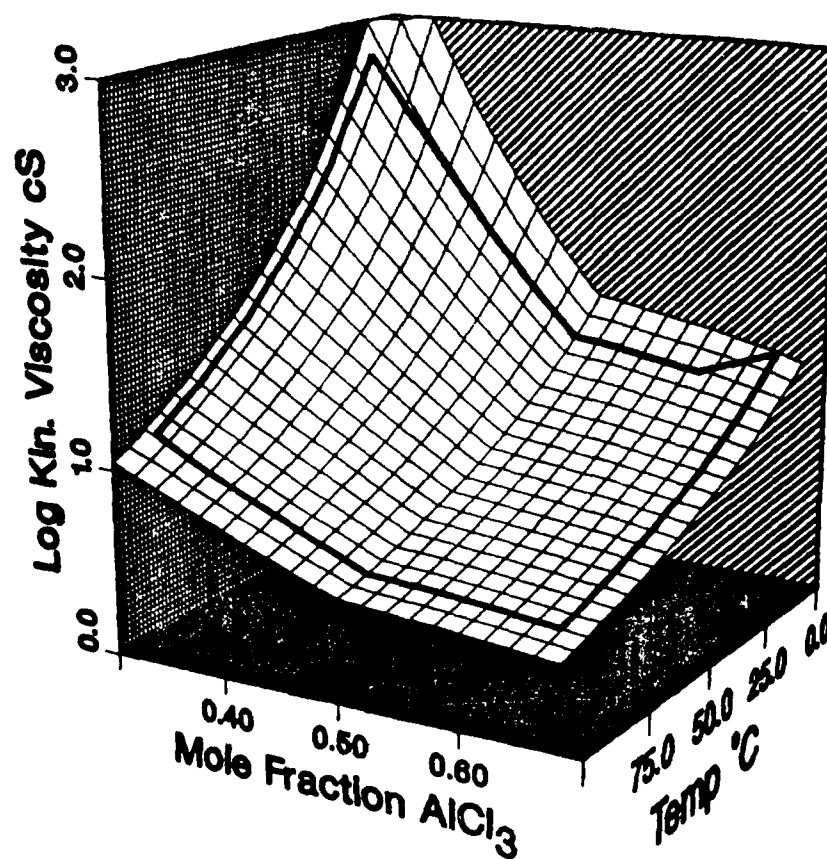


Figure 5

Melt Absolute Viscosity

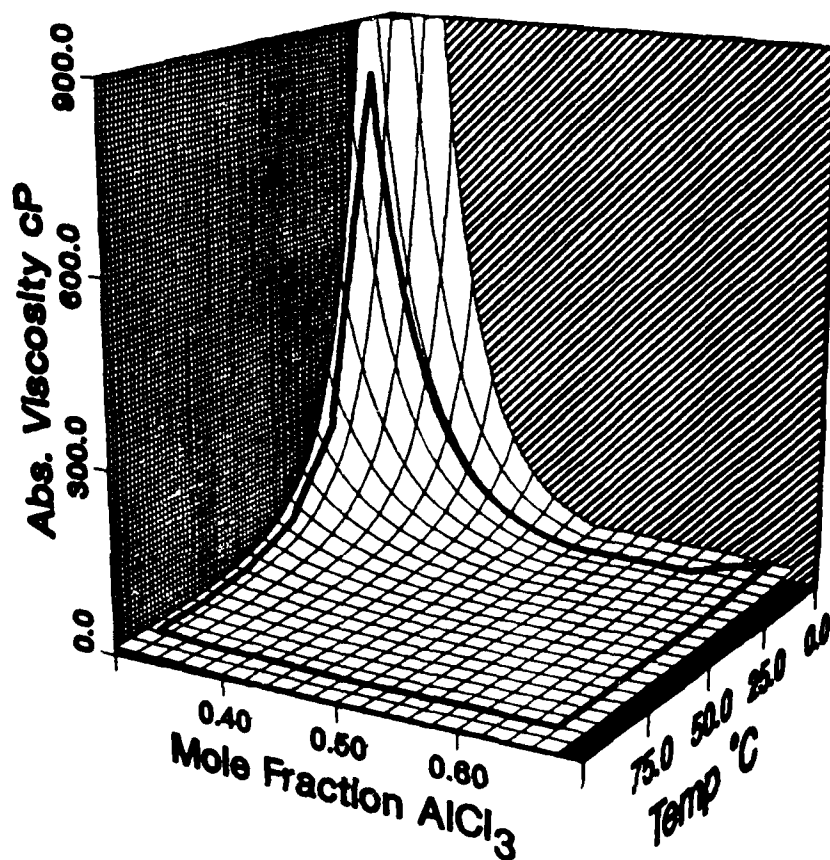


Figure 6

Melt Absolute Viscosity

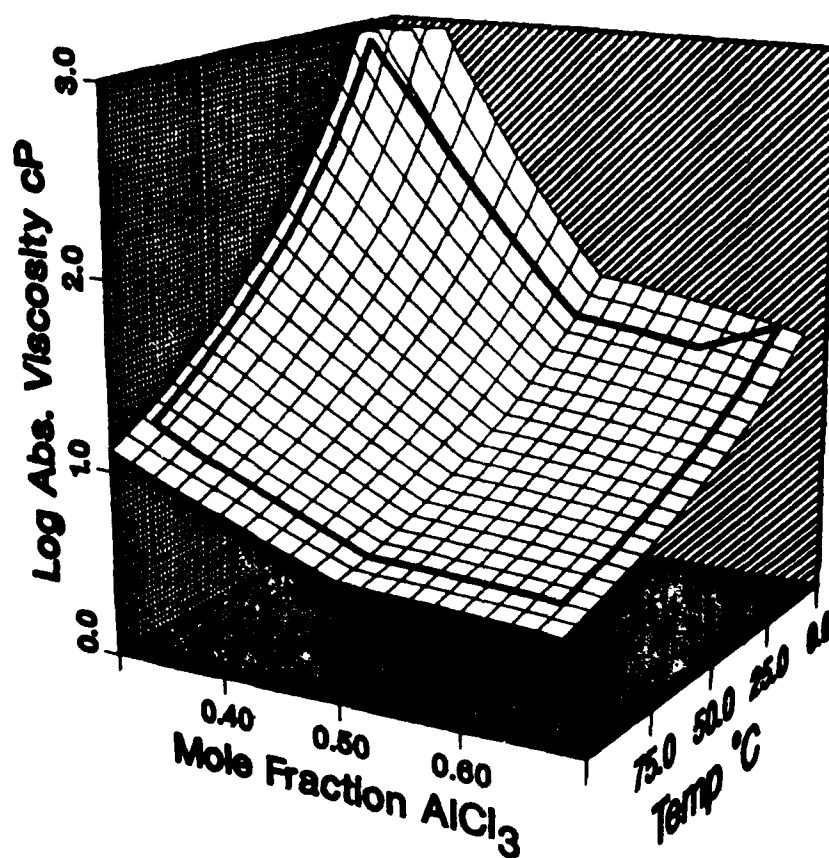


Figure 7

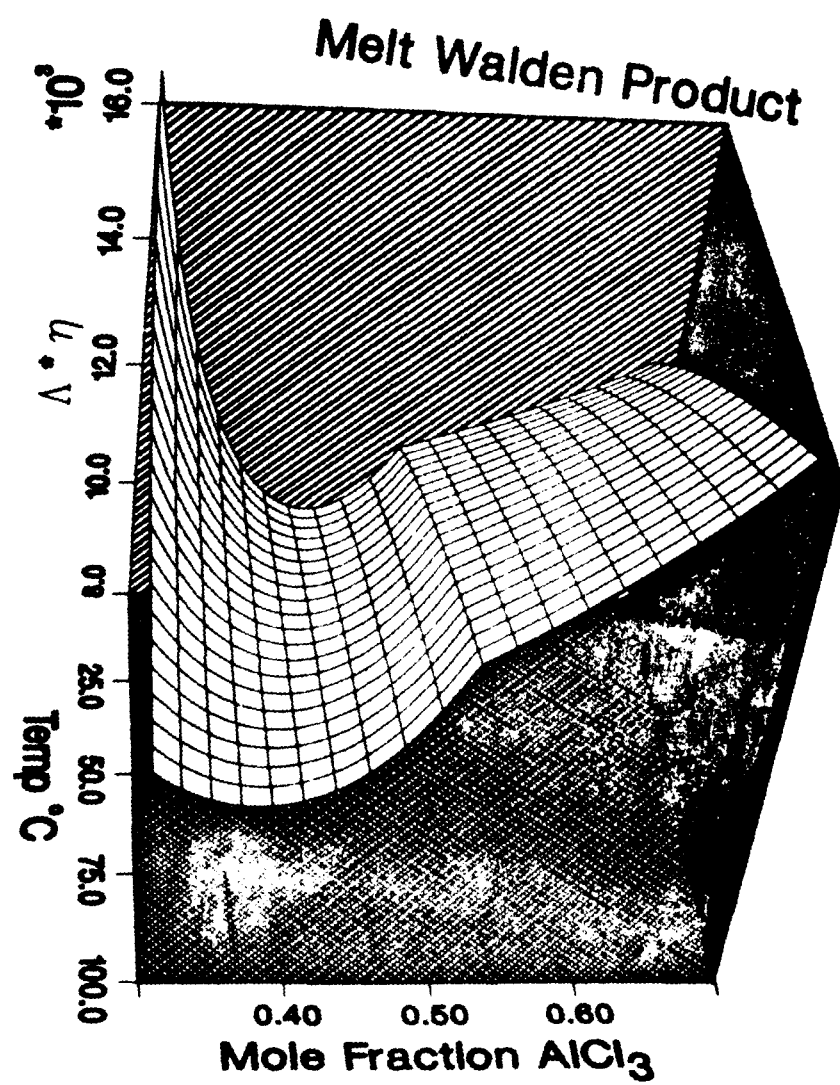


Figure 8

APPENDIX A

The FORTRAN programs for the different three-dimensional plots are largely the same. The principal differences are the function that generates the surface, the name of the data file containing the vertices of the polygon superimposed on the surface, the axes names and ranges and the view point.

A few comments about the programs are included here to simplify future use or modification for similar plots.

xx(min) etc.:	the minimum and maximum axes values
call ptek1:	Tektronix 4014 terminal as output device. The figures for this report were copied from a TEK 4014 screen, which has the highest resolution available at FJSRL and is much faster than a digital plotter.
call ptk41:	Tektronix 4107 as output device. Used for all but final copies. One or the other of these two calls is commented out.
call x3name etc.:	the axes labels
call vuang1:	establishes the viewpoint. The arguments are with respect to the center of the box containing the surface. The first argument is the angle (in the x-y or temperature-composition surface) from a line through the center of the box containing the surface parallel to the x (temperature) axis. The second argument is the angle up from the base plane (x,y). The third argument is the distance from the center.
call messag:	Early versions had messages printed on the box walls. These were commented out for the final copy.
call bshift:	moves the whole figure in x and y directions in order to get complete figure on screen.

ABSOLUTE VISCOSITY

```

external avis
integer tic
logical ok
dimension a(4),b(4),x(2),y(2),iabove(1)
dimension xx(3),yy(3),zz(3)
dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
data iabove/4HABOV/
min=1
max=2
tic=3
xx(min)=0.0
xx(max)=100.0
xx(tic)=25.0
yy(min)=0.301
yy(max)=0.70
yy(tic)=0.1
zz(max)=900.
zz(min)=0.0
zz(tic)=300.
call ldpoly(xpoly,ypoly,npoly)
c call ptk41
call ptek1
c call prpdev(ok)
c if(.not. ok) stop
c call hp7470
call hwrot('AUTO')
call swissm
call shdchr(90.,1,.002,1)
call height(.325)
call physor(.5,0.5)
call bshift(0.4,0.)
call nobrdr
call area2d(7.5,9.75)
x1=xmess('Melt Absolute Viscosity$',100)
call messag('Melt Absolute Viscosity$',100,4.0-x1/2.,9.25)
call volm3d(8.,8.,9.)
call mixalf('INSTRU')
call x3name('Temp (eh.5)o(exhx)C$',100)
call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
call z3name('Abs. Viscosity cP$',100)
call vuangl(30.,15.,40.)
call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
1 zz(min),zz(tic),zz(max))
call thkcrv(.05)
do 25 ii=1,npoly
call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25 call curv3d(xcrv,ycrv,zcrv,ncrv,0)
call blsur
call surfun(avis,5,xx(tic)*.2,5,yy(tic)*.2,0)
call grfitl(0.,0.,0.,0.,8.,0.,0.,0.,9.)
call area2d(8.,9.)
call cross
call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
call height(.525)

```

```

c  x1=xmess('A1C13$',100)
c  xpos=4.0-x1/2.
c  call messag('A1C13$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=yy(min)
  a(2)=yy(max)
  a(3)=yy(max)
  a(4)=yy(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=yy(min)
  x(2)=yy(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(19)
c  shadpat was 17
  call shdcrv(x,y,2,0,0,1above)
  call end3gr(0)
  call grfit1(0.,0.,0.,8.,0.,0.,8.,0.,9.)
  call area2d(8.,9.)
  call cross
  call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c  next 4 lines put msg on x-z wall
c  x1=xmess('deg C$',100)
c  xpos=4.0-x1/2.
c  call messag('deg C$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=xx(min)
  x(2)=xx(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(10)
c  shadpat was 18
  call shdcrv(x,y,2,0,0,1above)
  call end3gr(0)
  call grfit1(0.,0.,0.,8.,0.,0.,0.,8.,0.)
  call area2d(8.,8.)
  call cross
  call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)

```

```

b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function avis(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
  x2=(1.0-f)*(1.0-f)
  x5=2.0*f*(1.0-f)
  x11=0.0
  x14=0.0
else
  x2=0.0
  x5=0.0
  x14=(1.0-f)*(1.0-f)
  x11=2.0*f*(1.0-f)
endif
a2=252.3
a5=189.9
a8=142.2
a11=137.2
a14=132.2
b2=732.5
b5=0.
b8=0.
b11=0.
b14=0.
c2=-4.669
c5=0.
c8=0.
c11=0.
c14=0.
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
ck=732.5
aln=-4.669
z=ck/(ta-T0)+0.5*alog(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14

```

```

dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))
if (elamda.gt.900.) elamda=900.
avis=(elamda)
end
subroutine ldpoly(xpoly,ypoly,npoly)
dimension xpoly(*),ypoly(*)
open(unit=8,name='3dvis.dat',status='OLD',err=99)
do 10 i=1,100
read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10 npoly=npoly+1
20 write(5,'(2x,i4,' vertex polygon from 3dvis.dat ')') npoly
close(8)
return
99 write(5,'(' Error in reading 3Dvis.DAT file')')
stop
end
subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
nsegs=5
delta=1.0/nsegs
if(ii .ne. 1) then
x1=xpoly(ii-1)
y1=ypoly(ii-1)
else
x1=xpoly(npoly)
y1=ypoly(npoly)
end if
x2=xpoly(ii)
y2=ypoly(ii)
xx=x1
deltax=(x2-x1)*delta
yy=y1
deltay=(y2-y1)*delta
do 30 i=1,nsegs+1
xcrv(i)=xx
ycrv(i)=yy
zcrv(i)=avis(xx,yy)
xx=xx+deltax
30 yy=yy+deltay
ncrv=nsegs+1
return
end

```

SPECIFIC CONDUCTIVITY

```

external cond
integer tic
logical ok
dimension a(4),b(4),x(2),y(2),labove(1)
dimension xx(3),yy(3),zz(3)
dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
data labove/4HABOV/
min=1
max=2
tic=3
xx(min)=0.0
xx(max)=120.0
xx(tic)=30.0
yy(min)=0.0
yy(max)=0.70
yy(tic)=0.15
zz(max)=0.08
zz(min)=0.0
zz(tic)=.02
call ldpoly(xpoly,ypoly,npoly)
c call ptk41
call ptekal
c call prpdev(ok)
c if(.not. ok) stop
c call hp7470
call hwrot('AUTO')
call swissm
call shdchr(90.,1,.002,1)
call height(.325)
call physor(.5,0.5)
call bshift(0.3,0.)
call nobrdr
call area2d(7.5,9.75)
x1=xmess('Melt Specific Conductivity$',100)
call messag('Melt Specific Conductivity$',100,4.0-x1/2.,9.25)
call volm3d(8.,8.,9.)
call mixalf('INSTRU')
call x3name('Temp (eh.5)o(exhx)C$',100)
call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
call z3name('Sp. Cond. 1/ohm-cm$',100)
call vuangl(-13.,62.,40.)
call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
1 zz(min),zz(tic),zz(max))
call thkcrv(.05)
do 25 ii=1,npoly
call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25 call curv3d(xcrv,ycrv,zcrv,ncrv,0)
call blsur
call surfun(cond,5,xx(tic)*.2,5,yy(tic)*.2,0)
call grfitl(0.,0.,0.,0.,8.,0.,0.,0.,9.)
call area2d(8.,9.)
call cross
call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
call height(.525)
c x1=xmess('AlCl3$',100)

```

```

c  xpos=4.0-x1/2.
c  call messag('A1C13$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=yy(min)
  a(2)=yy(max)
  a(3)=yy(max)
  a(4)=yy(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=yy(min)
  x(2)=yy(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(19)
c  shadpat was 17
  call shdcrv(x,y,2,0,0,1,above)
  call end3gr(0)
  call grfit1(0.,8.,0.,8.,8.,0.,0.,8.,9.)
  call area2d(8.,9.)
  call cross
  call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c  next 4 lines put msg on x-z wall
c  x1=xmess('deg C$',100)
c  xpos=4.0-x1/2.
c  call messag('deg C$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=xx(min)
  x(2)=xx(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(10)
c  shadpat was 18
  call shdcrv(x,y,2,0,0,1,above)
  call end3gr(0)
  call grfit1(0.,0.,0.,8.,0.,0.,0.,8.,0.)
  call area2d(8.,8.)
  call cross
  call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)
  b(1)=yy(min)

```

```

b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,iabove)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function cond(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
    x2=(1.0-f)*(1.0-f)
    x5=2.0*f*(1.0-f)
    x11=0.0
    x14=0.0
else
    x2=0.0
    x5=0.0
    x14=(1.0-f)*(1.0-f)
    x11=2.0*f*(1.0-f)
endif
a2=259.9
a5=189.1
a8=123.4
a11=126.5
a14=121.9
b2=493.4
b5=763.0
b8=790.9
b11=802.1
b14=813.3
c2=8.0711
c5=8.7437
c8=8.9753
c11=8.9519
c14=8.9253
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
z=-ck/(ta-T0)-0.5*log(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))
cond=elamda*dense/em
end

```

```

subroutine ldpoly(xpoly,ypoly,npoly)
dimension xpoly(*),ypoly(*)
open(unit=8,name='3dCON.dat',status='OLD',err=99)
do 10 i=1,100
read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10 npoly=npoly+1
20 write(5,'(2x,14,' vertex polygon from 3dCON.dat ')) npoly
close(8)
return
99 write(5,'(' Error in reading 3dCON.DAT file'))
stop
end
subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
nsegs=5
delta=1.0/nsegs
if(ii .ne. 1) then
x1=xpoly(ii-1)
y1=ypoly(ii-1)
else
x1=xpoly(npoly)
y1=ypoly(npoly)
end if
x2=xpoly(ii)
y2=ypoly(ii)
xx=x1
deltax=(x2-x1)*delta
yy=y1
deltay=(y2-y1)*delta
do 30 i=1,nsegs+1
xcrv(i)=xx
ycrv(i)=yy
zcrv(i)=cond(xx,yy)
xx=xx+deltax
30 yy=yy+deltay
ncrv=ncrv+1
return
end

```

DENSITY

```

external dense
integer tic
logical ok
dimension a(4),b(4),x(2),y(2),labove(1)
dimension xx(3),yy(3),zz(3)
dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
data labove/4HABOV/
min=1
max=2
tic=3
xx(min)=5.0
xx(max)=95.0
xx(tic)=30.0
yy(min)=0.0
yy(max)=0.70
yy(tic)=0.15
zz(max)=1.50
zz(min)=1.00
zz(tic)=.1
call ldpoly(xpoly,ypoly,npoly)
C call ptk41
call ptekal
c call prpdev(ok)
c if(.not. ok) stop
c call hp7470
call hwrot('AUTO')
call swissm
call shdchr(90.,1,.002,1)
call height(.325)
call physor(.5,.625)
call area2d(7.5,9.75)
x1=xmess('Melt Density$',100)
call messag('Melt Density$',100,4.0-x1/2.,9.25)
call volm3d(8.,8.,9.)
call mixalf('INSTRU')
call x3name('Temp (eh.5)o(exhx)C$',100)
call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
call z3name('Density g/mL',12)
call vuangl(-30.,30.,30.)
call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
1 zz(min),zz(tic),zz(max))
call thkcrv(.05)
do 25 ii=1,npoly
call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25 call curv3d(xcrv,ycrv,zcrv,ncrv,0)
call blsur
call surfun(dense,5,xx(tic)*.2,5,yy(tic)*.2,0)
call grf1tl(0.,0.,0.,0.,8.,0.,0.,0.,9.)
call area2d(8.,9.)
call cross
call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
call height(.525)
x1=xmess('AlCl3$',100)
xpos=4.0-x1/2.

```

```

c  call messag('A1C13$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,xl+.2,.725,.02)
    a(1)=yy(min)
    a(2)=yy(max)
    a(3)=yy(max)
    a(4)=yy(min)
    b(1)=zz(min)
    b(2)=zz(min)
    b(3)=zz(max)
    b(4)=zz(max)
    x(1)=yy(min)
    x(2)=yy(max)
    y(1)=zz(min)
    y(2)=zz(min)
    call curve(a,b,4,0)
    call shdpat(19)
c  shadpat was 17
    call shdcrv(x,y,2,0,0,iabove)
    call end3gr(0)
    call grfiti(0.,8.,0.,8.,8.,0.,0.,8.,9.)
    call area2d(8.,9.)
    call cross
    call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c  next 4 lines put msg on x-z wall
c  x1=xmess('deg C$',100)
c  xpos=4.0-x1/2.
c  call messag('deg C$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,xl+.2,.725,.02)
    a(1)=xx(min)
    a(2)=xx(max)
    a(3)=xx(max)
    a(4)=xx(min)
    b(1)=zz(min)
    b(2)=zz(min)
    b(3)=zz(max)
    b(4)=zz(max)
    x(1)=xx(min)
    x(2)=xx(max)
    y(1)=zz(min)
    y(2)=zz(min)
    call curve(a,b,4,0)
    call shdpat(10)
c  shadpat was 18
    call shdcrv(x,y,2,0,0,iabove)
    call end3gr(0)
    call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
    call area2d(8.,8.)
    call cross
    call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
    a(1)=xx(min)
    a(2)=xx(max)
    a(3)=xx(max)
    a(4)=xx(min)
    b(1)=yy(min)
    b(2)=yy(min)

```

```

b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function dense(t,x)
f=1.0-abs((2*x-1)/(1-x))
tb=(t-60.0)*1.0e-4
x8=f*f
if(x.lt.0.5) then
  x2=(1.0-f)*(1.0-f)
  x5=2.0*f*(1.0-f)
  x11=0.0
  x14=0.0
else
  x2=0.0
  x5=0.0
  x14=(1.0-f)*(1.0-f)
  x11=2.0*f*(1.0-f)
endif
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
end
subroutine ldpoly(xpoly,ypoly,npoly)
dimension xpoly(*),ypoly(*)
open(unit=8,name='3dpoly.dat',status='OLD',err=99)
do 10 i=1,100
read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10 npoly=npoly+1
20 write(5,'(2x,14,' vertex polygon from 3dpoly.dat ')') npoly
close(8)
return
99 write(5,'(' Error in reading 3DPOLY.DAT file')')
stop
end
subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
nsegs=5
delta=1.0/nsegs
if(ii.ne.1) then
  x1=xpoly(ii-1)

```

```

        y1=ypoly(i1-1)
    else
        x1=xpoly(npoly)
        y1=ypoly(npoly)
    end if
    x2=xpoly(i1)
    y2=ypoly(i1)
    xx=x1
    deltax=(x2-x1)*delta
    yy=y1
    deltay=(y2-y1)*delta
    do 30 i=1,nsegs+1
        xcrv(i)=xx
        ycrv(i)=yy
        zcrv(i)=dense(xx,yy)
        xx=xx+deltax
30    yy=yy+deltay
        ncrv=nsegs+1
    return
end

```

EQUIVALENT CONDUCTIVITY

```

external cond
integer tic
logical ok
dimension a(4),b(4),x(2),y(2),labove(1)
dimension xx(3),yy(3),zz(3)
dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
data labove/4HABOV/
min=1
max=2
tic=3
xx(min)=0.0
xx(max)=120.0
xx(tic)=30.0
yy(min)=0.0
yy(max)=0.70
yy(tic)=0.15
zz(max)=20.
zz(min)=0.0
zz(tic)=5.
call ldpoly(xpoly,ypoly,npoly)
c call ptk41
call ptek1
c call prpdev(ok)
c if(.not. ok) stop
c call hp7470
call hwrot('AUTO')
call swissm
call shdchr(90.,1,.002,1)
call height(.325)
call physor(.5,0.5)
call bshift(0.3,0.)
call nobrdr
call area2d(7.5,9.75)
x1=xmess('Melt Equiv. Conductivity$',100)
call messag('Melt Equiv. Conductivity$',100,4.0-x1/2.,9.25)
call volm3d(8.,8.,9.)
call mixalf ('INSTRU')
call x3name('Temp (eh.5)o(exhx)C$',100)
call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
call z3name('Eq. Cond. cm(eh.5)2(hxex)/ohm-eq$',100)
call vuangl(-13.,62.,40.)
call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
1 zz(min),zz(tic),zz(max))
call thkcrv(.05)
do 25 ii=1,npoly
call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25 call curv3d(xcrv,ycrv,zcrv,ncrv,0)
call blsur
call surfun(cond,5,xx(tic)*.2,5,yy(tic)*.2,0)
call grfit1(0.,0.,0.,0.,8.,0.,0.,0.,9.)
call area2d(8.,9.)
call cross
call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
call height(.525)

```

```

c  x1=xmess('AlCl3$',100)
c  xpos=4.0-x1/2.
c  call messag('AlCl3$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=yy(min)
  a(2)=yy(max)
  a(3)=yy(max)
  a(4)=yy(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=yy(min)
  x(2)=yy(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(19)
c  shadpat was 17
  call shdcrv(x,y,2,0,0,1above)
  call end3gr(0)
  call grfit1(0.,8.,0.,8.,8.,0.,0.,8.,9.)
  call area2d(8.,9.)
  call cross
  call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c  next 4 lines put msg on x-z wall
c  x1=xmess('deg C$',100)
c  xpos=4.0-x1/2.
c  call messag('deg C$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=xx(min)
  x(2)=xx(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(10)
c  shadpat was 18
  call shdcrv(x,y,2,0,0,1above)
  call end3gr(0)
  call grfit1(0.,0.,0.,8.,0.,0.,0.,8.,0.)
  call area2d(8.,8.)
  call cross
  call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)

```

```

b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1,above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function cond(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
  x2=(1.0-f)*(1.0-f)
  x5=2.0*f*(1.0-f)
  x11=0.0
  x14=0.0
else
  x2=0.0
  x5=0.0
  x14=(1.0-f)*(1.0-f)
  x11=2.0*f*(1.0-f)
endif
a2=259.9
a5=189.1
a8=123.4
a11=126.5
a14=121.9
b2=493.4
b5=763.0
b8=790.9
b11=802.1
b14=813.3
c2=8.0711
c5=8.7437
c8=8.9753
c11=8.9519
c14=8.9253
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
z=-ck/(ta-T0)-0.5*a*log(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))

```

```

cond=elamda
end
subroutine ldpoly(xpoly,ypoly,npoly)
dimension xpoly(*),ypoly(*)
open(unit=8,name='3dCON.dat',status='OLD',err=99)
do 10 i=1,100
read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10 npoly=npoly+1
20 write(5,'(2x,i4,' vertex polygon from 3dCON.dat ')') npoly
close(8)
return
99 write(5,'(' Error in reading 3dCON.DAT file')')
stop
end
subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
nsegs=5
delta=1.0/nsegs
if(ii .ne. 1) then
x1=xpoly(ii-1)
y1=ypoly(ii-1)
else
x1=xpoly(npoly)
y1=ypoly(npoly)
end if
x2=xpoly(ii)
y2=ypoly(ii)
xx=x1
deltax=(x2-x1)*delta
yy=y1
deltay=(y2-y1)*delta
do 30 i=1,nsegs+1
xcrv(i)=xx
ycrv(i)=yy
zcrv(i)=cond(xx,yy)
xx=xx+deltax
30 yy=yy+deltay
ncrv=nsegs+1
return
end

```

KINEMATIC VISCOSITY

```

external avis
integer tic
logical ok
dimension a(4),b(4),x(2),y(2),labove(1)
dimension xx(3),yy(3),zz(3)
dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
data labove/4HABOV/
min=1
max=2
tic=3
xx(min)=0.0
xx(max)=100.0
xx(tic)=25.0
yy(min)=0.301
yy(max)=0.70
yy(tic)=0.1
zz(max)=3.
zz(min)=0.0
zz(tic)=1.
call ldpoly(xpoly,ypoly,npoly)
c call ptk41
c call ptekal
c call prpdev(ok)
c if(.not. ok) stop
c call hp7470
call hwrot('AUTO')
call swissm
call shdchr(90.,1,.002,1)
call height(.325)
call physor(.5,0.5)
call bshift(0.4,0.)
call nobrdr
call area2d(7.5,9.75)
x1=xmess('Melt Kinematic Viscosity$',100)
call messag('Melt Kinematic Viscosity$',100,4.0-x1/2.,9.25)
call volm3d(8.,8.,9.)
call mixalf('INSTRU')
call x3name('Temp (eh.5)o(exhx)C$',100)
call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
call z3name('Log Kin. Viscosity cS$',100)
call vuangl(30.,15.,40.)
call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
1 zz(min),zz(tic),zz(max))
call thkcrv(.05)
do 25 ii=1,npoly
call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25 call curv3d(xcrv,ycrv,zcrv,ncrv,0)
call blsur
call surfun(avis,5,xx(tic)*.2,5,yy(tic)*.2,0)
call grfit1(0.,0.,0.,0.,8.,0.,0.,0.,9.)
call area2d(8.,9.)
call cross
call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
call height(.525)

```

```

c  x1=xmess('AlCl3$',100)
c  xpos=4.0-x1/2.
c  call messag('AlCl3$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=yy(min)
  a(2)=yy(max)
  a(3)=yy(max)
  a(4)=yy(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=yy(min)
  x(2)=yy(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(19)
c  shadpat was 17
  call shdcrv(x,y,2,0,0,1above)
  call end3gr(0)
  call grfiti(0.,0.,0.,8.,0.,0.,8.,0.,9.)
  call area2d(8.,9.)
  call cross
  call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c  next 4 lines put msg on x-z wall
c  x1=xmess('deg C$',100)
c  xpos=4.0-x1/2.
c  call messag('deg C$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)
  b(1)=zz(min)
  b(2)=zz(min)
  b(3)=zz(max)
  b(4)=zz(max)
  x(1)=xx(min)
  x(2)=xx(max)
  y(1)=zz(min)
  y(2)=zz(min)
  call curve(a,b,4,0)
  call shdpat(10)
c  shadpat was 18
  call shdcrv(x,y,2,0,0,1above)
  call end3gr(0)
  call grfiti(0.,0.,0.,8.,0.,0.,8.,0.)
  call area2d(8.,8.)
  call cross
  call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
  a(1)=xx(min)
  a(2)=xx(max)
  a(3)=xx(max)
  a(4)=xx(min)

```

```

b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,iabove)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function avis(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
    x2=(1.0-f)*(1.0-f)
    x5=2.0*f*(1.0-f)
    x11=0.0
    x14=0.0
else
    x2=0.0
    x5=0.0
    x14=(1.0-f)*(1.0-f)
    x11=2.0*f*(1.0-f)
endif
a2=252.3
a5=189.9
a8=142.2
a11=137.2
a14=132.2
b2=732.5
b5=0.
b8=0.
b11=0.
b14=0.
c2=-4.669
c5=0.
c8=0.
c11=0.
c14=0.
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
ck=732.5
aln=-4.669
z=ck/(ta-T0)+0.5*log(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
de=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14

```

```

dense=de-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))
elamda=elamda/dense
if (elamda.gt.1000.) elamda=1000.
avis=alog10(elamda)
end
subroutine ldpoly(xpoly,ypoly,npoly)
dimension xpoly(*),ypoly(*)
open(unit=8,name='3dvis.dat',status='OLD',err=99)
do 10 i=1,100
read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10 npoly=npoly+1
20 write(5,'(2x,i4,' vertex polygon from 3dvis.dat ')') npoly
close(8)
return
99 write(5,'(' Error in reading 3Dvis.DAT file')')
stop
end
subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
nsegs=5
delta=1.0/nsegs
if(ii .ne. 1) then
x1=xpoly(ii-1)
y1=ypoly(ii-1)
else
x1=xpoly(npoly)
y1=ypoly(npoly)
end if
x2=xpoly(ii)
y2=ypoly(ii)
xx=x1
deltax=(x2-x1)*delta
yy=y1
deltay=(y2-y1)*delta
do 30 i=1,nsegs+1
xcrv(i)=xx
ycrv(i)=yy
zcrv(i)=avis(xx,yy)
xx=xx+deltax
30 yy=yy+deltay
ncrv=nsegs+1
return
end

```

WALDEN PRODUCT

```

external wald
integer tic
logical ok
dimension a(4),b(4),x(2),y(2),labove(1)
dimension xx(3),yy(3),zz(3)
dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
data labove/4HABOV/
min=1
max=2
tic=3
xx(min)=0.0
xx(max)=100.0
xx(tic)=25.0
yy(min)=0.301
yy(max)=0.70
yy(tic)=0.1
zz(max)=16000.
zz(min)=8000.0
zz(tic)=2000.
c call ldpoly(xpoly,ypoly,npoly)
c call ptk41
c call ptek1
c call prpdev(ok)
c if(.not. ok) stop
c call hp7470
c call hwrot('AUTO')
c call swissm
c call shdchr(90.,1,.002,1)
c call height(.325)
c call physor(.5,0.5)
c call bshift(0.3,0.)
c call nobrdr
c call area2d(7.5,9.75)
x1=xmess('Melt Walden Product$',100)
c call messag('Melt Walden Product$',100,4.0-x1/2.,9.25)
c call volm3d(8.,8.,9.)
c call mixalf('INSTRU')
c call x3name('Temp (eh.5)o(exhx)C$',100)
c call y3name('Mole Fraction AlCl(1.5)3(lx)C$',100)
c call z3name('(m6)L(mx) * (m7)c(mx)C$',100)
c call vuangl(-11.,40.,40.)
c call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
1 zz(min),zz(tic),zz(max))
c call thkcrv(.05)
do 25 ii=1,npoly
c call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25 c call curv3d(xcrv,ycrv,zcrv,ncrv,0)
c call blsur
c call surfun(wald,5,xx(tic)*.2,5,yy(tic)*.2,0)
c call grfit1(0.,0.,0.,0.,8.,0.,0.,0.,9.)
c call area2d(8.,9.)
c call cross
c call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
c call height(.525)

```

```

c  x1=xmess('A1C13$',100)
c  xpos=4.0-x1/2.
c  call messag('A1C13$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
    a(1)=yy(min)
    a(2)=yy(max)
    a(3)=yy(max)
    a(4)=yy(min)
    b(1)=zz(min)
    b(2)=zz(min)
    b(3)=zz(max)
    b(4)=zz(max)
    x(1)=yy(min)
    x(2)=yy(max)
    y(1)=zz(min)
    y(2)=zz(min)
    call curve(a,b,4,0)
    call shdpat(19)
c  shadpat was 17
    call shdcrv(x,y,2,0,0,1,above)
    call end3gr(0)
    call grfit1(0.,8.,0.,8.,8.,0.,0.,8.,9.)
    call area2d(8.,9.)
    call cross
    call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c  next 4 lines put msg on x-z wall
c  x1=xmess('deg C$',100)
c  xpos=4.0-x1/2.
c  call messag('deg C$',100,xpos,7.)
c  call blrec(xpos-.1,6.9,x1+.2,.725,.02)
    a(1)=xx(min)
    a(2)=xx(max)
    a(3)=xx(max)
    a(4)=xx(min)
    b(1)=zz(min)
    b(2)=zz(min)
    b(3)=zz(max)
    b(4)=zz(max)
    x(1)=xx(min)
    x(2)=xx(max)
    y(1)=zz(min)
    y(2)=zz(min)
    call curve(a,b,4,0)
    call shdpat(10)
c  shadpat was 18
    call shdcrv(x,y,2,0,0,1,above)
    call end3gr(0)
    call grfit1(0.,0.,0.,8.,0.,0.,0.,8.,0.)
    call area2d(8.,8.)
    call cross
    call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
    a(1)=xx(min)
    a(2)=xx(max)
    a(3)=xx(max)
    a(4)=xx(min)

```

```

b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function wald(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
  x2=(1.0-f)*(1.0-f)
  x5=2.0*f*(1.0-f)
  x11=0.0
  x14=0.0
else
  x2=0.0
  x5=0.0
  x14=(1.0-f)*(1.0-f)
  x11=2.0*f*(1.0-f)
endif
a2=259.9
a5=189.1
a8=123.4
a11=126.5
a14=121.9
b2=493.4
b5=763.0
b8=790.9
b11=802.1
b14=813.3
c2=8.0711
c5=8.7437
c8=8.9753
c11=8.9519
c14=8.9253
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
z=-ck/(ta-T0)-0.5*a*log(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))

```

```

    elamda=elamda*em/dense
    av2=252.3
    av5=189.9
    av8=142.2
    av11=137.2
    av14=132.2
    etak=732.5
    etaaln=-4.669
    etaT0=x2*av2+x5*av5+av8*x8+av11*x11+av14*x14
    avis=exp(etak/(ta-T0)+0.5*log(ta)+etaaln)
    wald=min(elamda*avis,20000.)
    end
    subroutine ldpoly(xpoly,ypoly,npoly)
    dimension xpoly(*),ypoly(*)
    open(unit=8,name='3dCON.dat',status='OLD',err=99)
    do 10 i=1,100
    read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
    write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10  npoly=i
20  write(5,'(2x,i4,' ' vertex polygon from 3dCON.dat '))'') npoly
    close(8)
    return
99  write(5,'(' ' Error in reading 3dCON.DAT file'))'')
    stop
    end
    subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
    dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
    nsegs=5
    delta=1.0/nsegs
    if (ii .ne. 1) then
        x1=xpoly(ii-1)
        y1=ypoly(ii-1)
    else
        x1=xpoly(npoly)
        y1=ypoly(npoly)
    end if
    x2=xpoly(ii)
    y2=ypoly(ii)
    xx=x1
    deltax=(x2-x1)*delta
    yy=y1
    deltay=(y2-y1)*delta
    do 30 i=1,nsegs+1
    xcrv(i)=xx
    ycrv(i)=yy
    zcrv(i)=wald(xx,yy)
    xx=xx+deltax
30  yy=yy+deltay
    ncrv=nsegs+1
    return
    end

```

APPENDIX B

THREE-DIMENSIONAL EQUATIONS FOR MeEtImCl-AlCl₃ BINARY MELTS

DENSITY: g/cm³ [Valid for $0.25 \leq N \leq 0.6666$ and $10^\circ\text{C} \leq t \leq 90^\circ\text{C}$]

$$\rho = \frac{X_2 a_2 + X_5 a_5 + X_8 a_8 + X_{11} a_{11} + X_{14} a_{14} + (X_2 b_2 + X_5 b_5 + X_8 b_8 + X_{11} b_{11} + X_{14} b_{14}) (t - 60)}{(1)} \quad (1)$$

where the a_i 's and b_i 's represent the parameters in the equation below for the individual "complexes" with 2, 5, 8, 11, and 14 chlorides.

$$\rho = a + b (t - 60) \quad (2)$$

The X_i 's may be calculated most conveniently as follows: Let f be the anion fraction of AlCl_4^- . Then $f = 1 - |(2N - 1)/(1 - N)|$. For $0 < N < 0.5$, $X_2 = (1 - f)^2$, $X_5 = 2f(1 - f)$, and X_{11} and $X_{14} = 0$. For $0.5 < N \leq 0.667$, X_2 and $X_5 = 0$, $X_{11} = 2f(1 - f)$, and $X_{14} = (1 - f)^2$. At all compositions $X_8 = f^2$.

TABLE I. Least Squares Fitted Parameters for Equation 1 Densities.^a

i	a_i	$-b_i \times 10^4$
2	1.1279	6.1096
5	1.2208	6.6170
8	1.2662	8.0153
11	1.3263	8.7004
14	1.3567	9.1690

^a The parameters yield $\sigma = 0.0004$ in ρ , where $\sigma = [\Sigma(\rho_{\text{calc}} - \rho_{\text{exp}})^2 / (\text{number of points} - \text{number of fitted parameters})]^{1/2}$.

CONDUCTIVITY: $\text{cm}^2/\text{eq/L}$ [Valid for $0.30 \leq N \leq 0.6666$ and $20^\circ\text{C} \leq t \leq 100^\circ\text{C}$]

VISCOSITY: cP [Valid for $0.31 \leq N \leq 0.6666$ and $10^\circ\text{C} \leq t \leq 90^\circ\text{C}$]

$$\ln \Lambda = -\underline{k}_\Lambda / (\underline{T} - \underline{T}_0) - 1/2 \ln \underline{T} + \ln \underline{A}_\Lambda \quad (3)$$

and

$$\ln \eta = \underline{k}_\eta / (\underline{T} - \underline{T}_0) + 1/2 \ln \underline{T} + \ln \underline{A}_\eta \quad (4)$$

where

$$\underline{T}_0 = \underline{X}_2 \underline{a}_2 + \underline{X}_5 \underline{a}_5 + \underline{X}_8 \underline{a}_8 + \underline{X}_{11} \underline{a}_{11} + \underline{X}_{14} \underline{a}_{14} \quad (5)$$

$$\underline{k} = \underline{X}_2 \underline{b}_2 + \underline{X}_5 \underline{b}_5 + \underline{X}_8 \underline{b}_8 + \underline{X}_{11} \underline{b}_{11} + \underline{X}_{14} \underline{b}_{14} \quad (6)$$

$$\ln \underline{A} = \underline{X}_2 \underline{c}_2 + \underline{X}_5 \underline{c}_5 + \underline{X}_8 \underline{c}_8 + \underline{X}_{11} \underline{c}_{11} + \underline{X}_{14} \underline{c}_{14} \quad (7)$$

where the \underline{a} 's, \underline{b} 's, and \underline{c} 's represent the \underline{T}_0 , \underline{k}_Λ and $\ln \underline{A}_\Lambda$, respectively, for each of the individual "complexes" with 2, 5, 8, 11, and 14 chlorides.

The \underline{X}_i 's are calculated as given for densities.

TABLE II. Least Squares Fitted Parameters for Equations 3, 4 and 5-7 Equivalent Conductivities and Absolute Viscosities of 1-Methyl-3-ethylimidazolium Chloride - Aluminum Chloride Binary Mixtures

Eq 3 or 4 Parameters	Equations 5-7 "complex" species parameter				
	2	5	8	11	14
Eq 3 and 5-7 Parameters for Equivalent Conductivity ^a					
$\underline{T}_0, \text{K}$	259.5	189.1	123.4	126.5	121.9
$\underline{k}_\Lambda, \text{K}$	493.4	763.0	790.9	802.1	813.3
$\ln \underline{A}_\Lambda$	8.0711	8.7437	8.9753	8.9519	8.9253
Eq 4 and 5-7 Parameters for Absolute Viscosity ^b					
$\underline{T}_0, \text{K}$	252.3	189.9	142.2	137.2	132.2
$\underline{k}_\eta, \text{K}$	732.5 ^c				
$\ln \underline{A}_\eta$	-4.669 ^c				

^a The parameters yield $\sigma = 0.02$ in $\ln \Lambda$, where $\sigma = [\sum (\ln \Lambda_{\text{calc}} - \ln \Lambda_{\text{exp}})^2 / (\text{number of points} - \text{number of fitted parameters})]^{1/2}$.

^b The parameters yield $\sigma = 0.03$ in $\ln \eta$, where $\sigma = [\sum (\ln \eta_{\text{calc}} - \ln \eta_{\text{exp}})^2 / (\text{number of points} - \text{number of fitted parameters})]^{1/2}$.

^c These values are not parameters but averaged values of \underline{k}_η and $\ln \underline{A}_\eta$ to be used for absolute viscosity calculations at all compositions.

END

10-87

DTIC